Fumaric acid, naphth-2-yl 2-ethylhexyl ester

Inchi: InChI=1S/C22H26O4/c1-3-5-8-17(4-2)16-25-21(23)13-14-22(24)26-20-12-11-18-9-6-7-10
InchiKey: GSKZDCPRCVIIGF-BUHFOSPRSA-N
Formula: C22H26O4
SMILES: CCCCC(CC)COC(=O)C=CC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-46.27	kJ/mol	Joback Method
hf	-458.94	kJ/mol	Joback Method
hfus	45.66	kJ/mol	Joback Method
hvap	87.03	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.061		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1460.13	kPa	Joback Method
rinpol	2824.00		NIST Webbook
rinpol	2824.00		NIST Webbook
tb	909.70	K	Joback Method
tc	1129.77	K	Joback Method
tf	533.58	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.64	J/mol×K	909.70	Joback Method
cpg	907.34	J/mol×K	946.38	Joback Method
cpg	921.00	J/mol×K	983.06	Joback Method
cpg	933.69	J/mol×K	1019.74	Joback Method
cpg	945.48	J/mol×K	1056.41	Joback Method
cpg	956.46	J/mol×K	1093.09	Joback Method
cpg	966.69	J/mol×K	1129.77	Joback Method
dvisc	0.0005922	Pa×s	533.58	Joback Method

dvisc	0.0003399	Pa×s	596.27	Joback Method
dvisc	0.0002169	Pa×s	658.95	Joback Method
dvisc	0.0001496	Pa×s	721.64	Joback Method
dvisc	0.0001095	Pa×s	784.33	Joback Method
dvisc	0.0000839	Pa×s	847.01	Joback Method
dvisc	0.0000667	Pa×s	909.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405831&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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